Shortening the Insertion Time for Materials Technologies— the 21st Century Metals Challenge

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Standard Form 298 (Rev. 8-98)
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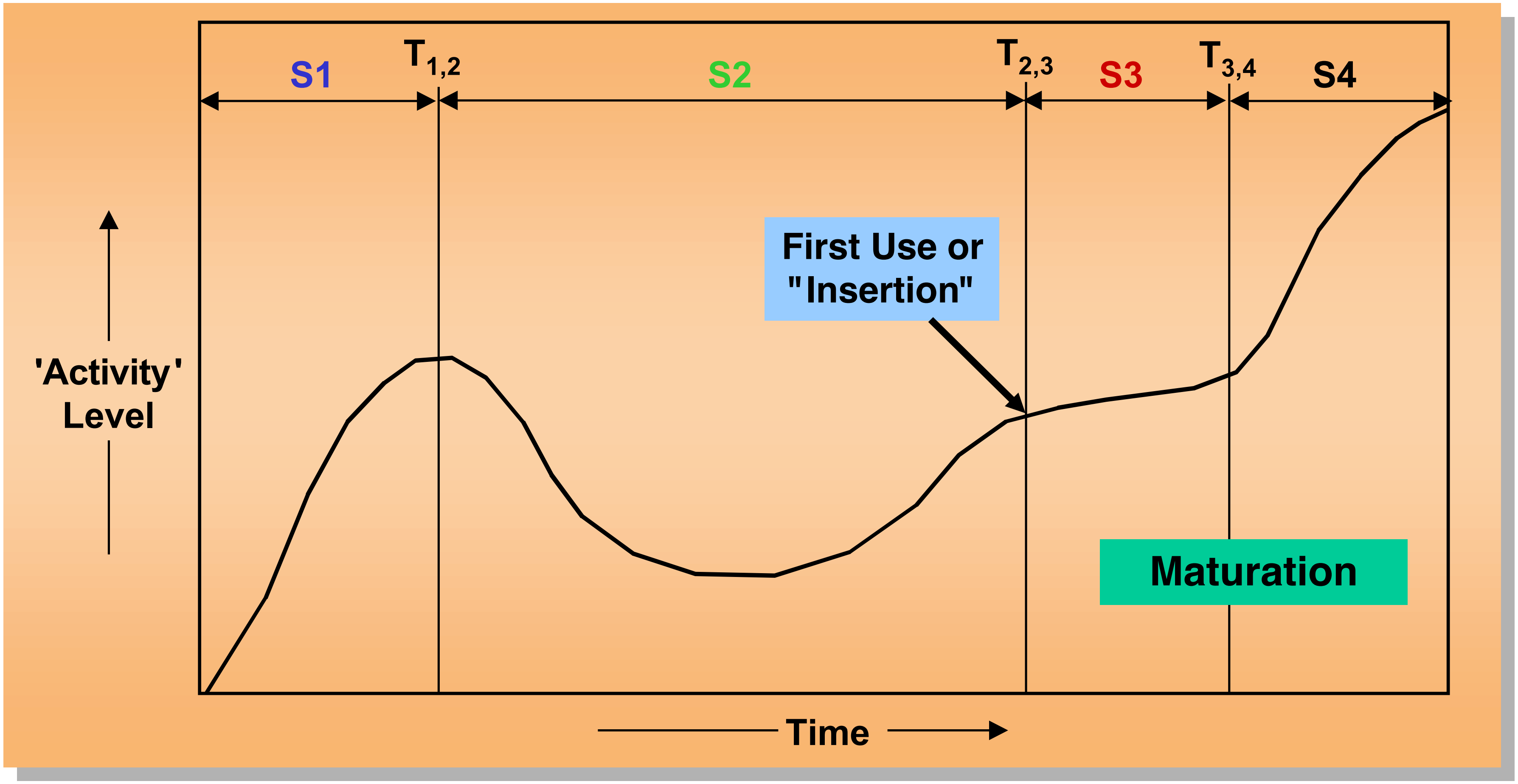
Observation: Historical Aerospace Material Life Cycle



Stages

S1 = Revolutionary

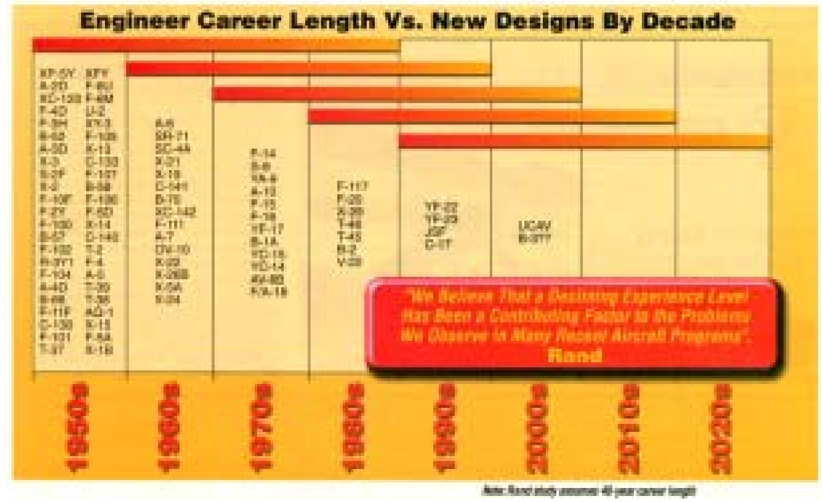
S2 = Emerging

S3 = Specialty Material

S4 = Commodity Material

Aerospace Structural Materials Development: How It Happened

Adapted from Fraser, 1998; Wax, 1999



- DoD materials transition opportunities (systems) have drastically reduced
- Material development time far exceeds the modern short product cycle
  - iterative, empirical development of "Knowledge Base" is lengthy, data intensive, and expensive

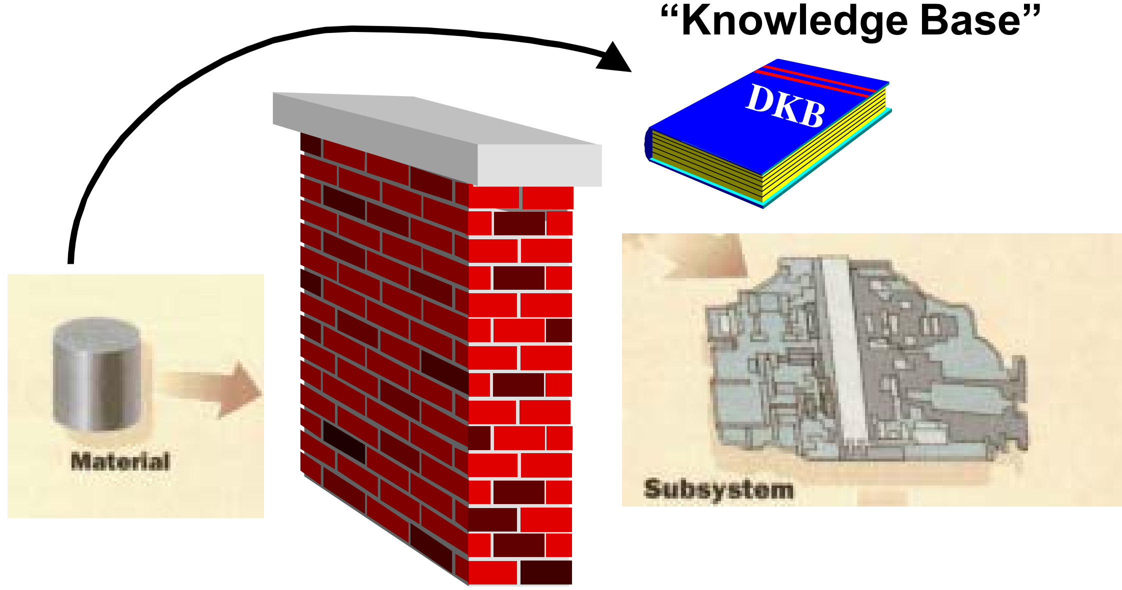
21st Century Reality Demands that the Paradigm Change!

The Disconnect!

Major disconnect between materials development & components/systems engineering design

- Known alloy to reliable part ~36 months
- Steels for navy landing gear 15+ yrs
- Lightweight composites for army vehicles 15+ yrs
- Gamma titanium aluminides ~30yrs and counting
- Ceramics for engines - 30+++ ? yrs
- Evolutionary alloy changes (ship steels, superalloys, etc) ~7-10 years

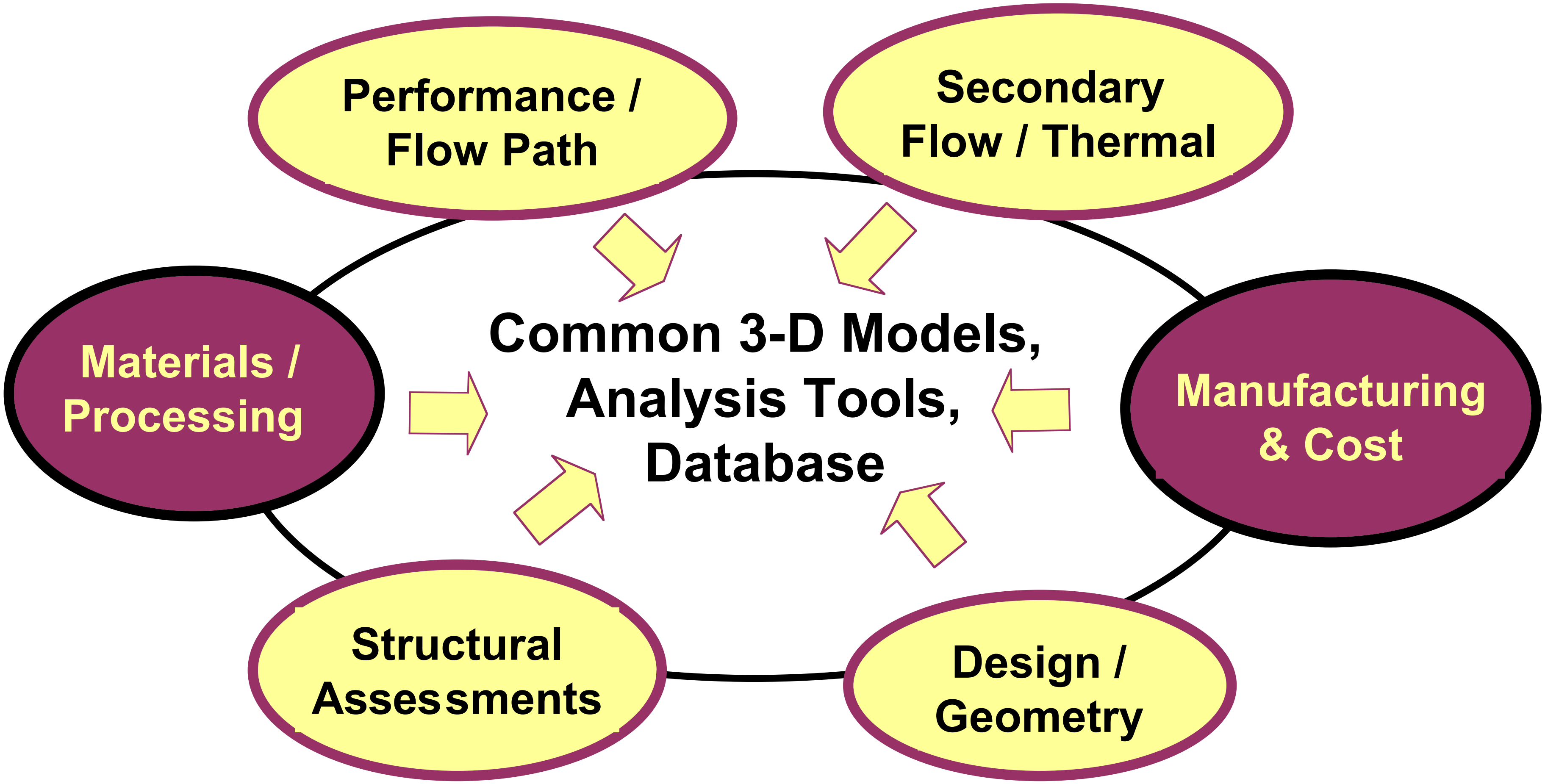
Materials
“Knowledge Base”



Materials Development
- Highly Empirical
- Testing Independent of Use
- Existing Models Unlinked

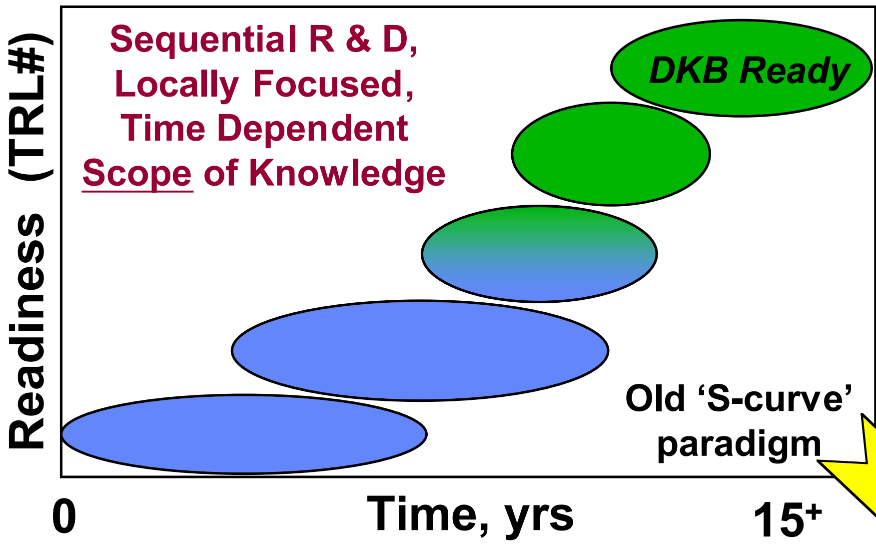
Engineering Design
- Materials Input from “Knowledge Base” of Data (Data Sheets, Graphs, Heuristics, Experience, etc.)
- System/Sub-System Design is Heavily Computational and Rapid
- Well Established Testing Protocols

Integrating Materials & Processes with Engine Design



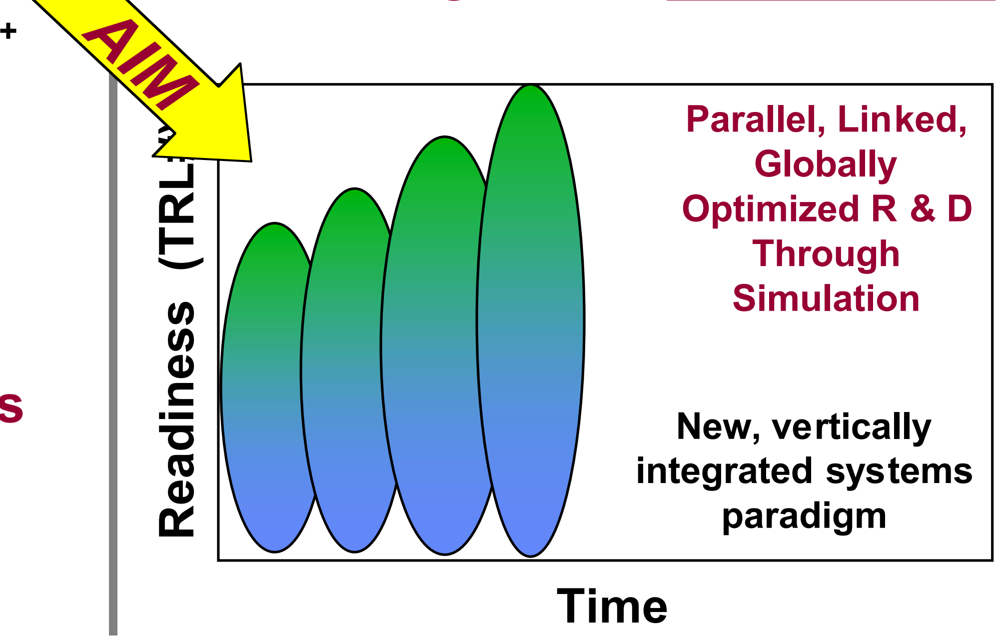
Design "development cycle": <3 yrs	Materials & Process "cycle": 7-20 yrs

AIM Paradigm for Materials R & D

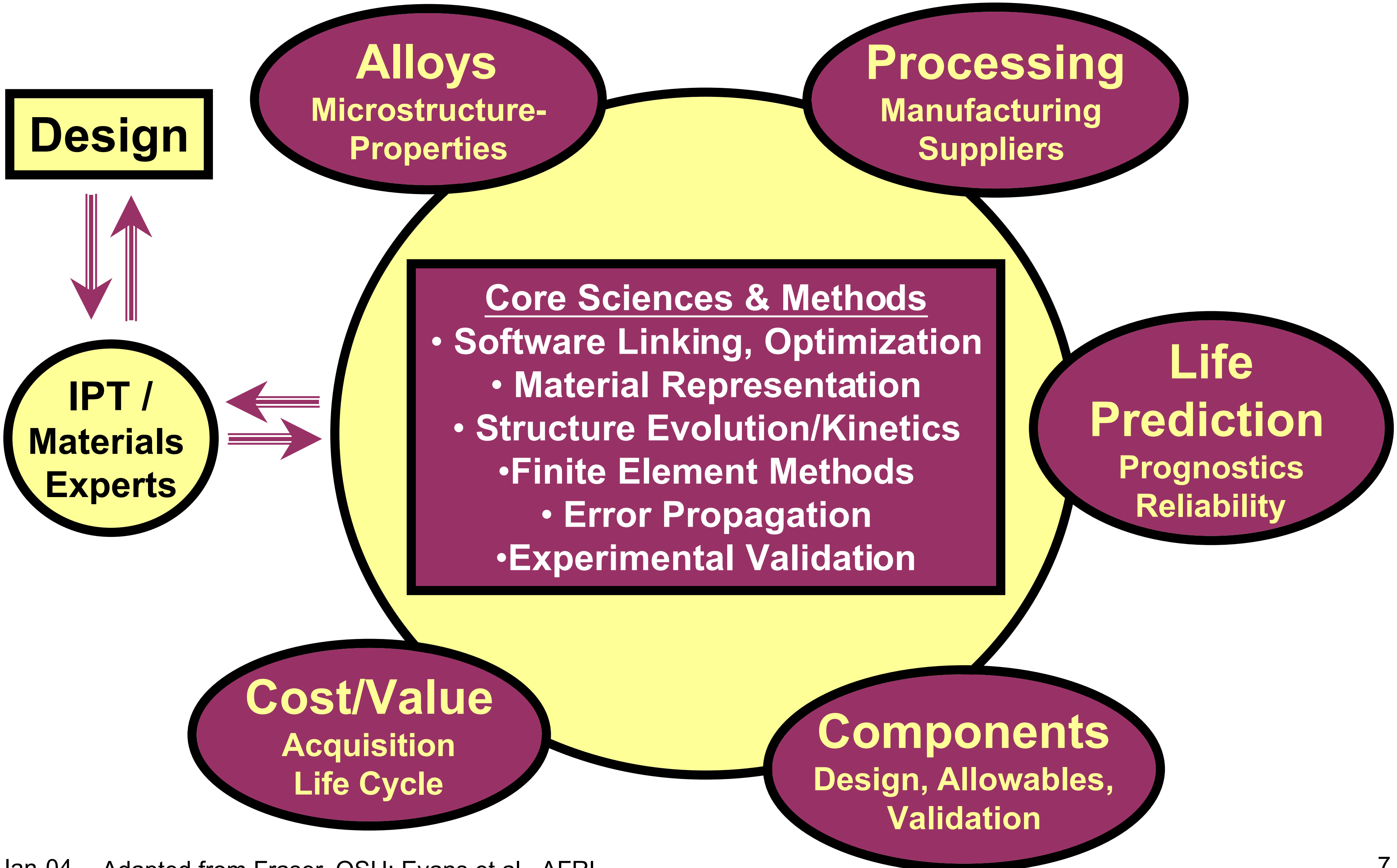


- Sequential M & P
- Optimized from heuristics
- "Designer Knowledge Base" NOT Ready Until Final Stages

- Building "Designer Knowledge Base" begins at outset
- Optimization based on <u>design IPT need</u>
- Time & effort refines <u>quality</u> of knowledge base, <u>not its scope</u>



Major Components of Designer Knowledge Base



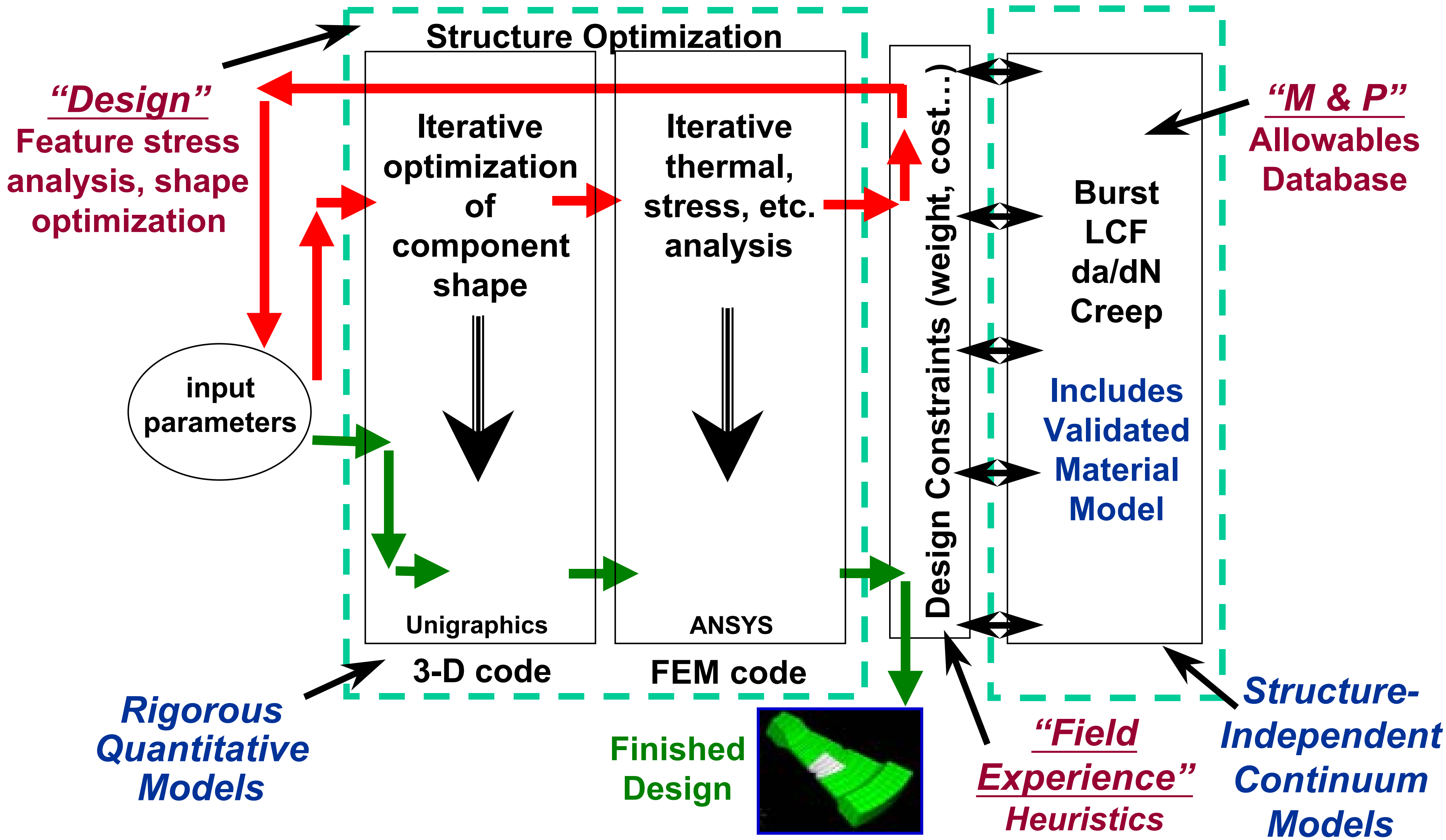
 Adapted from Fraser, OSU; Evans et al., AFRL

Guiding Constraints

- **A key deliverable must be a validated representation of the material and process: *designers work with representations!***
- **Structural materials design demands confidence in *control of time-dependent properties*, thus representations needed for**
  - **LCF, HCF, crack growth**
  - **creep, stress rupture**
  - **environmental degradation, stress corrosion**
  - **friction, wear, and fretting**
- ***'New material' demands rapid, validated representations*—but how?**
- **Need *ubiquitous tools* for optimization:**
  - ***a representation framework***
  - ***efficient validation***

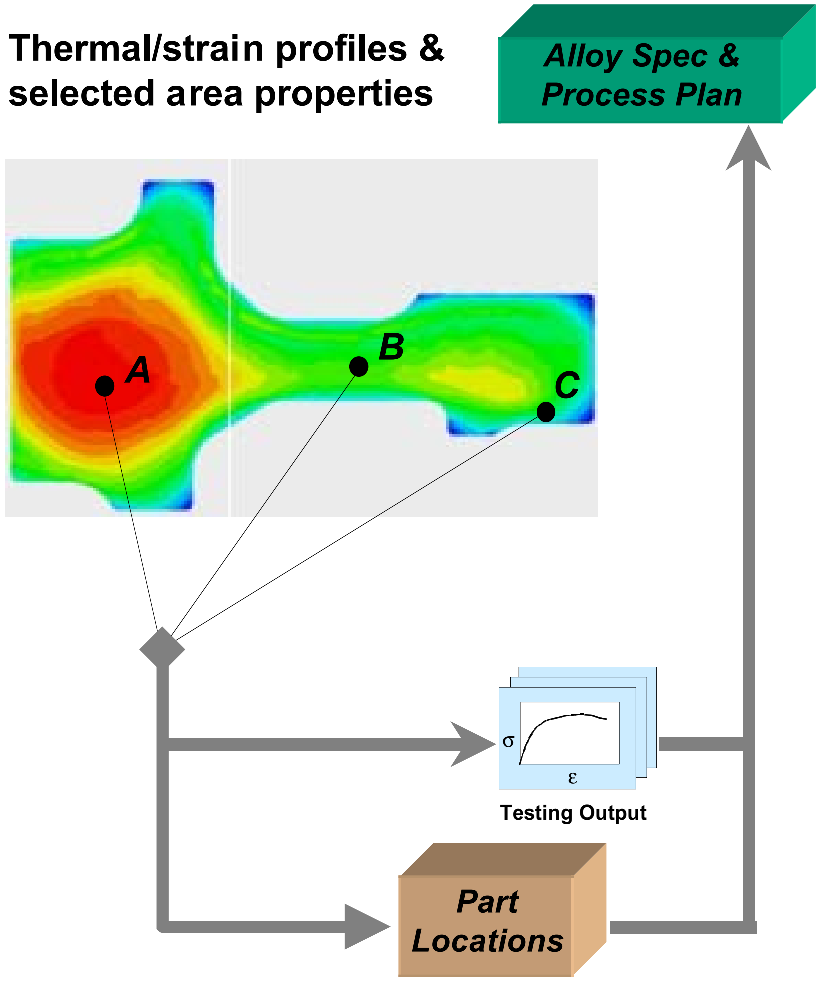
'Accelerated Insertion' Rather Than 'Materials by Design'

Modeling in the Component Design Process



"Field Experience" corrects for i) microstructure variation, ii) inaccurate analysis, & iii) incomplete understanding of service environment

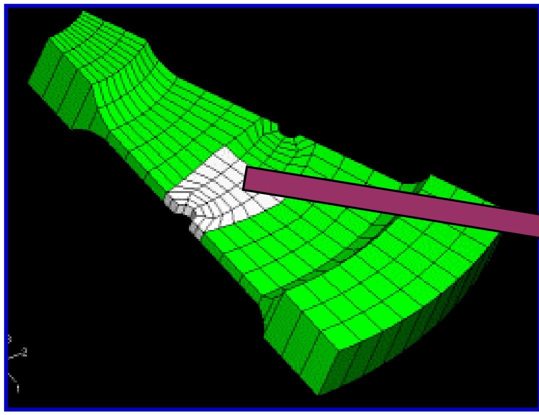
The Case of Ni-Alloy Engine Disks



- Continuum codes (i.e., DEFORM) for thermal history and microstructure correlation over disk cross-section
- Cross-section may be "zoned" into a few regions (dual heat treat); *centimeter-scale homogenization*
- *Empirical* yield-strength models, & flow-curve 'templates,' used to assign constitutive response
- Variation of structure averaged out; *local microstructure - defect interactions not represented*
- *Data-intensive* and time-costly process for yield model and 'constitutive template' validation

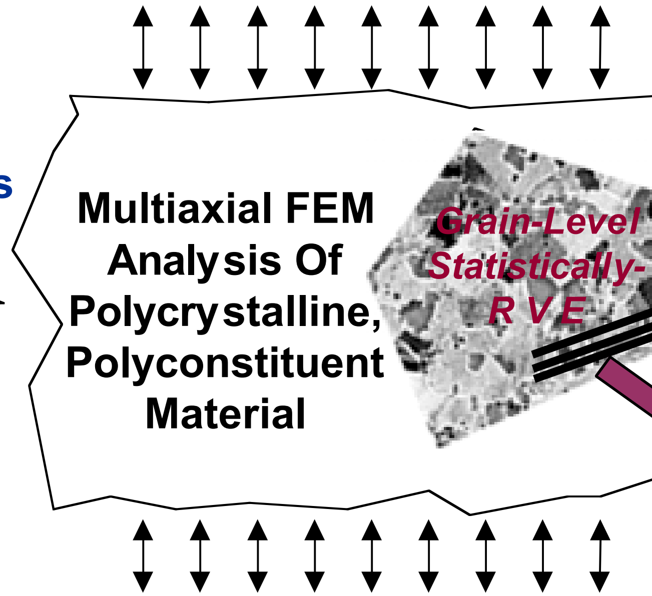
Challenges to represent time-dependent failure; to introduce "new material"

The "Plasticity Engine" for Properties

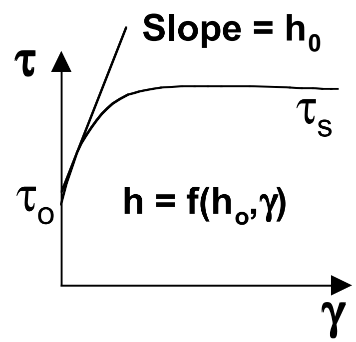


Design Concept

Define Features



Plastic Heterogeneity & Strain Localization



Focus on Work-Hardening Parameterization *With μ/s Effects*

$$\dot{\tau} = \left\{ h - \left(\frac{\tau - \tau_o}{\tau_s - \tau_o} \right) h \right\} \left(\dot{\gamma} / \dot{\gamma}_o \right)^m$$

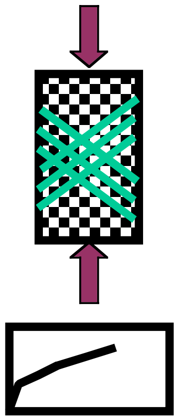
Properties of Representative Volume Element

Conventional Finite Element Model	$\{\tau_o, \tau_s, m, h\}$
Continuum Crystal Plasticity	$\{\tau_{o,i}, \tau_{s,i}, m, h_{ij}\}$
Constrained Crystal Plasticity	$\{\tau_{o,i}(k_{hp}), \tau_{s,i}, m, h_{ij}\}$
Strain-Gradient Crystal Plasticity	$\{\tau_{o,i}, \tau_{s,i}, m, h_{ij}\} + k_o$

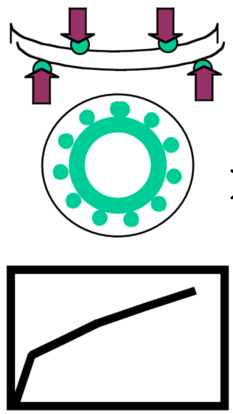
must define $\tau(\rho)$, $\rho(\gamma)$ to find k_o

increasing granularity & compute complexity

Build from Uni- / Multiaxial Slip & Work Hardening



uniaxial, crystal test



multiaxial, gradient test

Microstrain Experiments

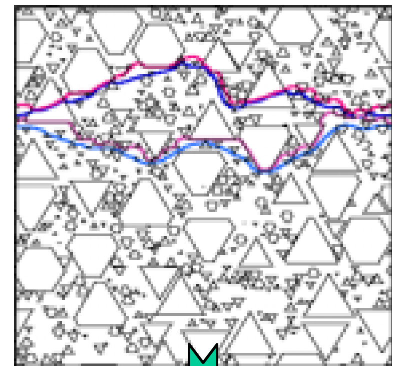
for single-, poly- &
polycrystalline slip

Microstructure Representation

characterize precipitate shape parameter and size/spacing distribution, etc.

Dislocation Kinetics Simulations

Intrinsic length effects, strain gradients



Compare

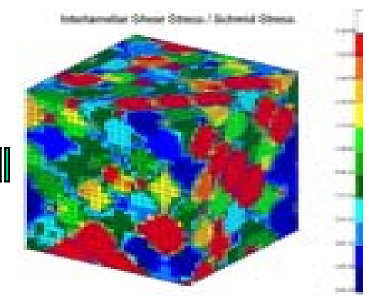
Existing links too weak

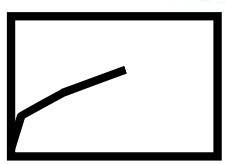
Numerical/Analytical Model

Representation of
work-hardening from
microstructure variation

~ <10 μm^3, 3-D

Scientific Frontier





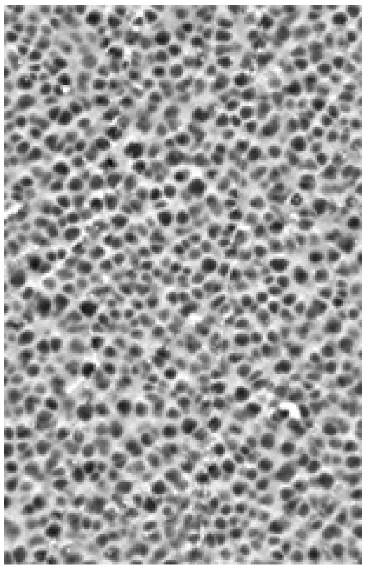
Predicted RVE Response

Single-slip & latent-hardening constitutive law for single-crystals; constitutive laws for polycrystalline RVEs (UMATs for 'intrinsic material' RVEs)

Direct links: computationally challenging & underdeveloped

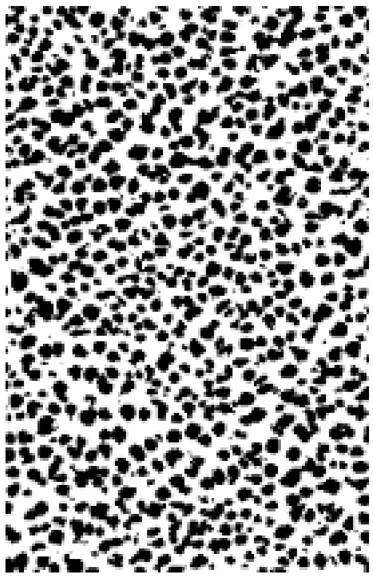
Real Microstructure in Simulations

TIFF
Image (PC)



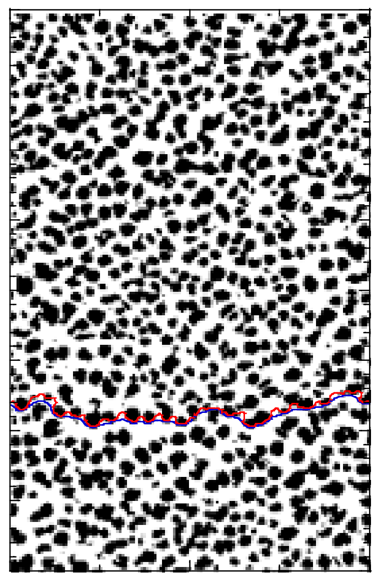
Rene88DT-Bore
2.5 x 4 μm
(BEI - S. Menon)

Binary
Image
(PC)

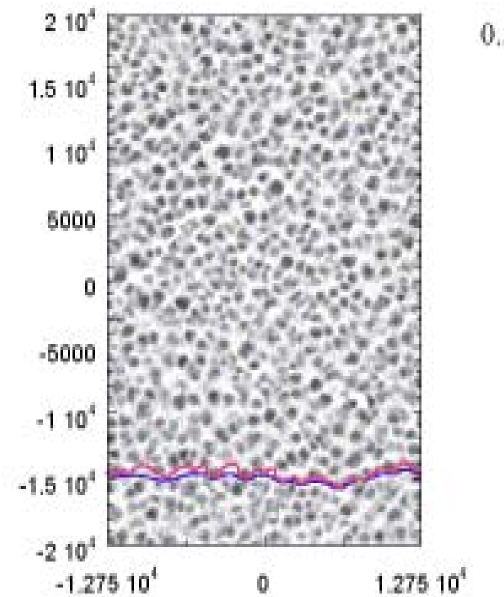


Simulation (Unix)
(pseudo-periodic)

τ =290 MPa



Simulation
superposed on
Microstructure

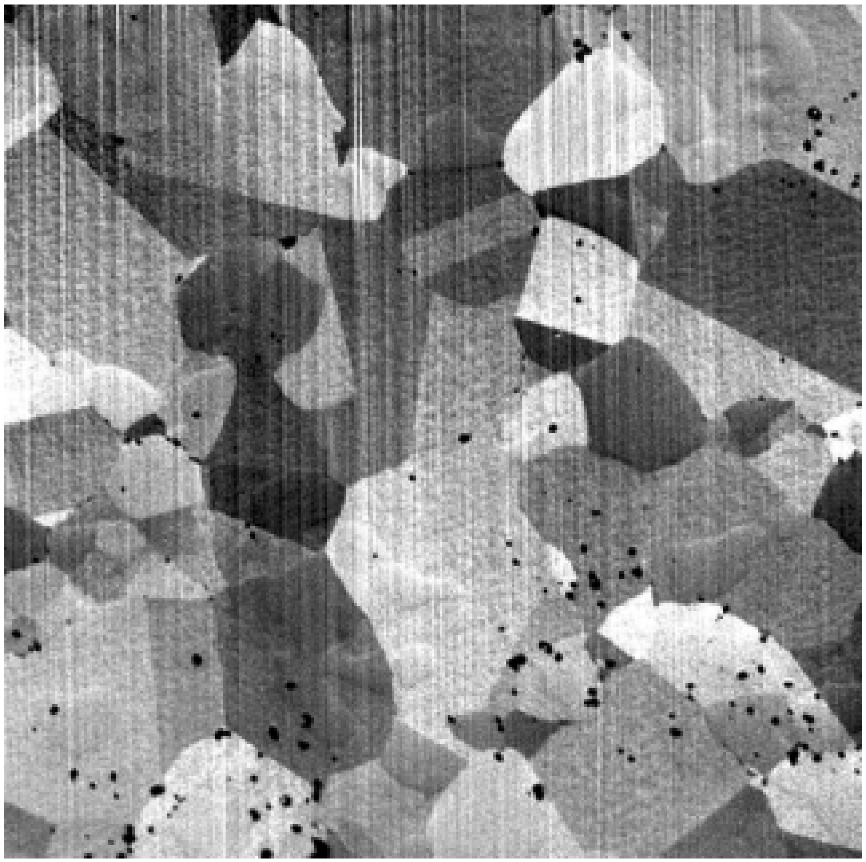


τ =290 MPa

Rao, Parthasarathy, Menon, Dimiduk & Hazzledine, 2002

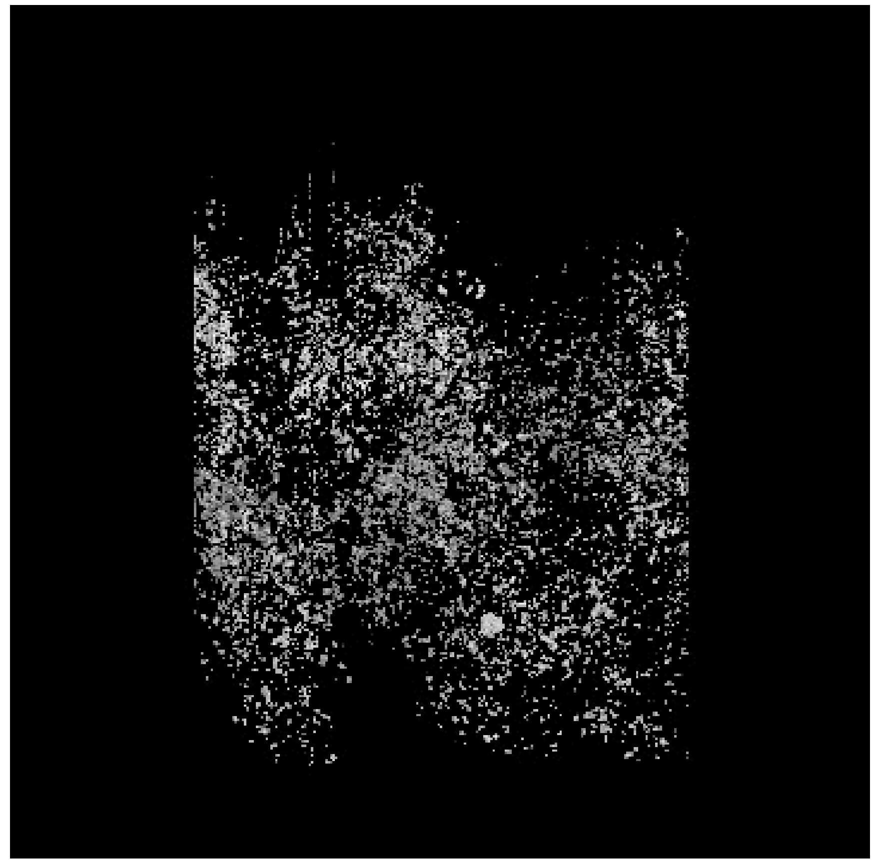
3-D Quantitative Microscopy

Serial Sectioning & Imaging



5 µm

3-D Rendering of Structure

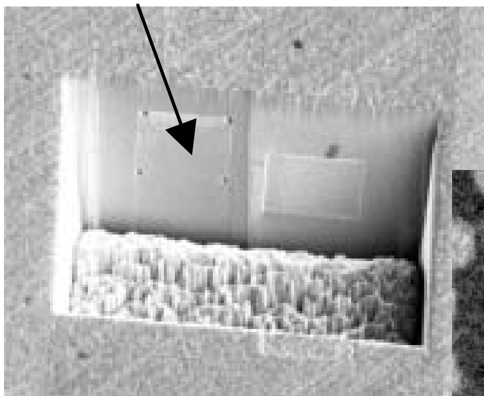


IN-100 Ni-base Superalloy
Grain Structure and Carbide/Boride Distribution

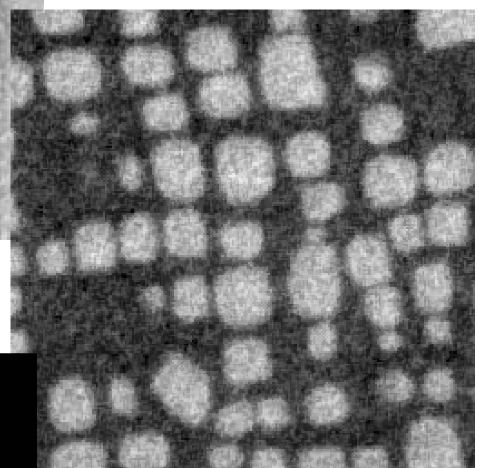
3-D Quantitative Microscopy

Serial Sectioning & Imaging

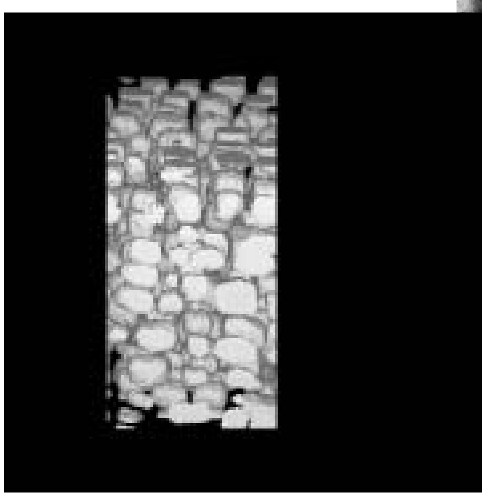
14 x 14 μm Image Area



Ni-Cr-Al Superalloy



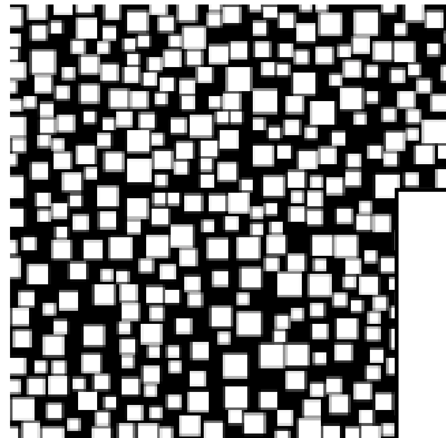
Aligned stack (~20 nm spacing)

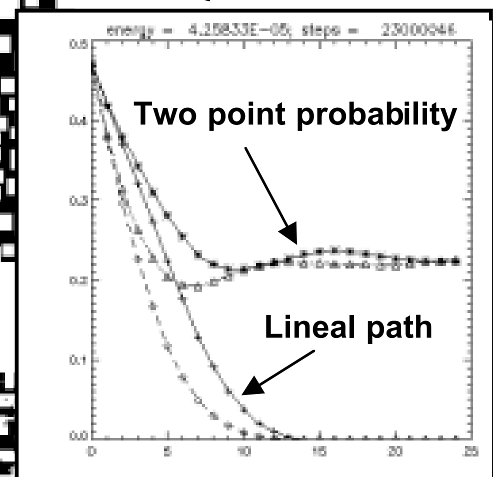


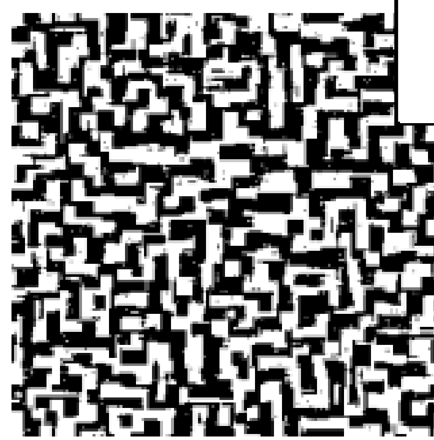
Rendered 3-D volume (~3 μm thick)

Mathematical Representation

Idealized Microstructure



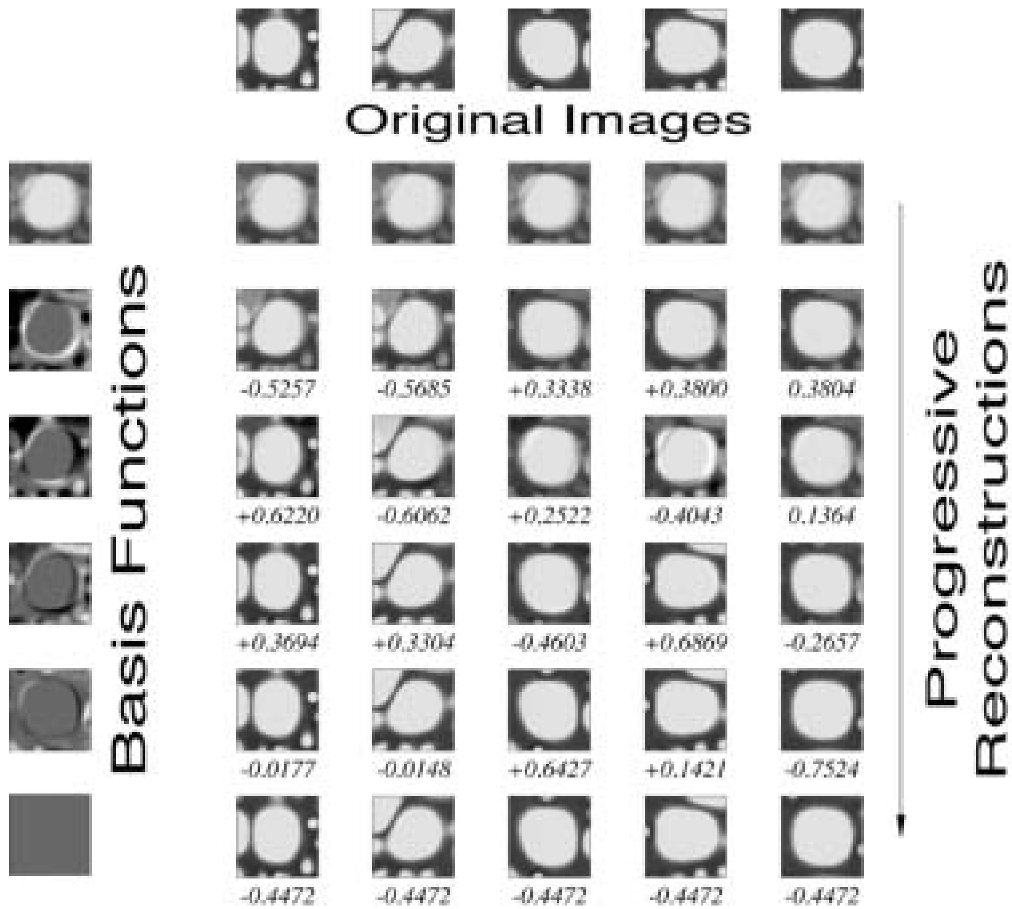




Monte Carlo Reconstructed Representative Microstructure

Uchic, Wheeler, Simmons, DeGraef & Dimiduk, 2001

Principal Component Analysis of Microstructure

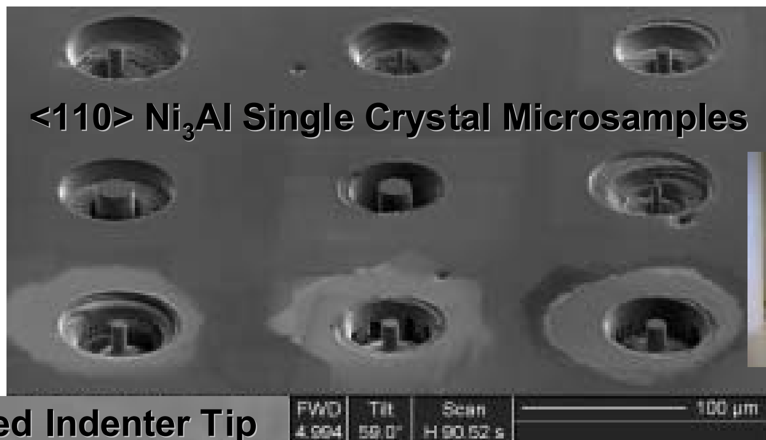


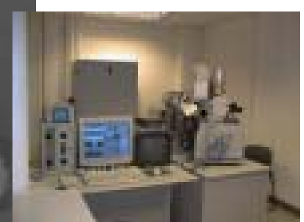
Representation Coefficients

-0.5257	-0.5685	0.3338	0.3800	0.3804
0.6220	-0.6062	0.2522	-0.4043	0.1364
0.3694	0.3304	-0.4603	0.6869	-0.2657
-0.0177	-0.0148	0.6427	0.1421	-0.7524
-0.4472	-0.4472	-0.4472	-0.4472	-0.4472

Mechanical Testing of Ultra-Small Samples for Crystal Properties

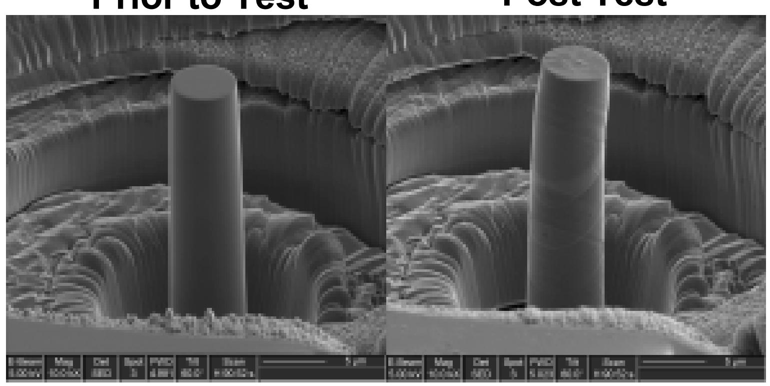
- *Focus efforts on linking simulation to design*
- *Small-scale properties measurement for constitutive representations*
- *Theory for broad understanding of deformation at small scales*

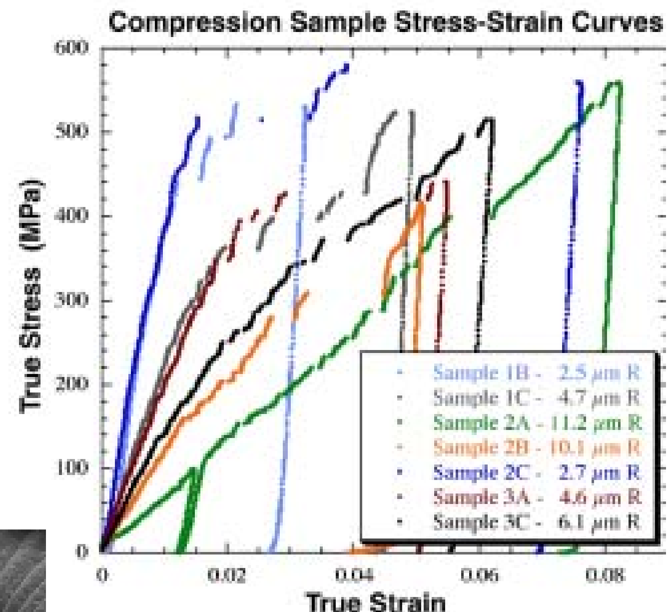




Prior to Test

Post Test

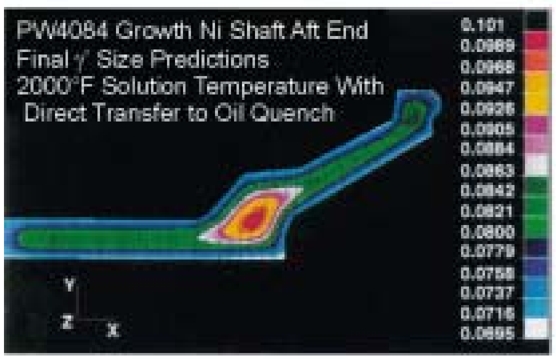


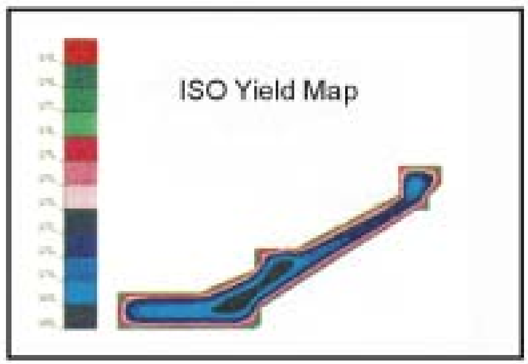


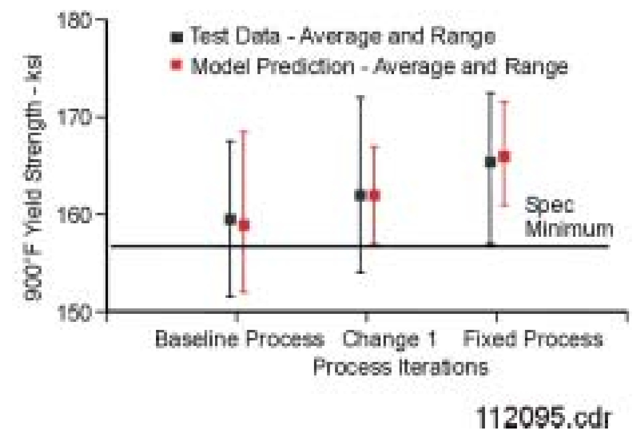
 Uchic, Dimiduk, Florando & Nix, 2002

Even Simple Models Have a <u>Big</u> Impact

- **Integrated structure-property-process models successfully applied as <u>point</u> solutions**
  - **statistically fit data to mechanistic-based property model**
  - **focused experiments to model microstructural evolution**
  - **accurate estimate of *mean* behavior**







P & W →

Shaft design:
- 1/4 development time
- 80% reduction in cost

Experience shows concept is <u>sound</u>, projected payoffs <u>reasonable</u>

Eventually Must Address Full Breadth of Component Requirements

<u>Requirements for Turbine Engine Disks</u>:

- ***Ultimate Tensile Strength***
- ***0.2 % Yield Strength***
- ***Tensile Ductilities***
- ***Notch Strength***
- ***Burst Margin***
- ***Creep***
- ***Rupture***
- ***Rupture Ductilities***
- **Continuous Cycling LCF**
- **Hold Time LCF**
- **Continuous Cycling Crack Growth**
- **Hold Time Crack Growth**
- **Superplasticity**
- **Flow Stresses**
- **Abnormal Grain Growth Resistance**
- **Gamma Prime Solvus**
- **Carbide(s) Solvus**
- **Density**

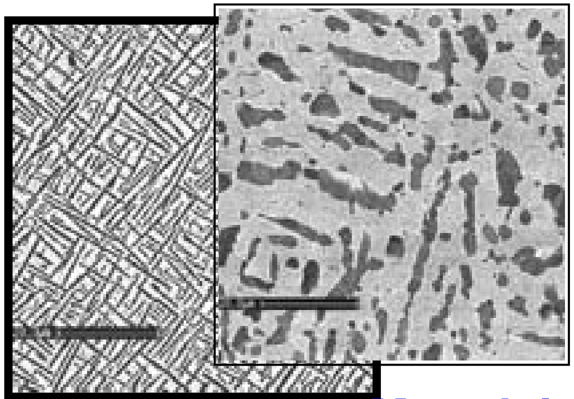
<u>DARPA - AIM</u>

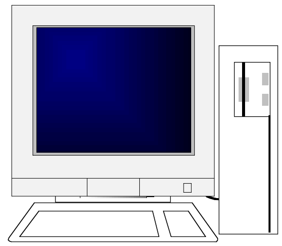
- **TIP**
- **Structural Stability**
- **Exposed Behavior**
- **Defect Sensitivity**
- **Defect Content**
- **Grain Size**
- **Gamma Prime Size**
- **Segregation /Effects**
- ***Inspectibility***
- ***Quench Crack Resistance***
- ***Multi-source Capability***
- ***Low Costs--Elemental and Processing***
- ***Weldability***
- ***Machinability***
- ***Machined Surface Behavior***
- ***Residual Stresses***
- ***Cost Reduction Potential***
- ***Size/Volume Scaling Effects***

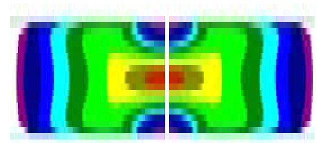
The <u>Issues</u> That Often Determine <u>Success or Failure</u>

Materials & System Readiness

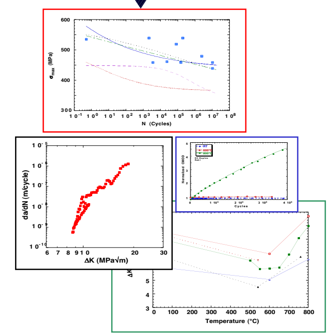
AIM







Materials Mathematics Experiment Experience



Property Database

Mathematics

State Awareness

Failure Physics

Data Fusion

Reasoning System

Prognostics

Combat System Readiness

Summary

- The *time* for structural materials development and use must be shortened (time focus, not cost focus)

- Industrial M & P community demanding a quantum-leap in *relevant engineering simulation* capability

- *Accelerated Insertion of Materials* is the long-term, strategically-relevant, computational materials science & engineering vision

- Materials Science & Engineering community must produce *integrated predictive tools*

- Accelerated insertion demands *integration of* engineering *design with M & P* to achieve true systems engineering of materials technologies